

Deriving the Gross-Pitaevskii equation

Niels Benedikter

Institute of Applied Mathematics, University of Bonn
Endenicher Allee 60, 53115 Bonn, Germany
E-mail: niels.benedikter@tofoq.de

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Abstract

In experiments, Bose-Einstein condensates are prepared by cooling a dilute Bose gas in a trap. After the phase transition has been reached, the trap is switched off and the evolution of the condensate observed. The evolution is macroscopically described by the Gross-Pitaevskii equation. On the microscopic level, the dynamics of Bose gases are described by the N -body Schrödinger equation. We review our article [BdS12] in which we construct a class of initial data in Fock space which are energetically close to the ground state and prove that their evolution approximately follows the Gross-Pitaevskii equation. The key idea is to model two-particle correlations with a Bogoliubov transformation.

Keywords: Bose-Einstein condensate; dilute Bose gas; Gross-Pitaevskii equation; correlations; many-body systems; Bogoliubov transformations; squeezed coherent states.

1 Bose-Einstein condensates in the Gross-Pitaevskii regime

In dilute gases of bosonic particles, at very low temperatures a phase transition occurs and a macroscopic number of particles occupies the same one-particle state. Bose and Einstein theoretically predicted this state of matter in 1924, considering non-interacting bosons. The experimental confirmation took 70 years and was rewarded with a Nobel prize in 2001, and the theoretical study of interacting Bose-Einstein condensates still poses challenging problems.

A dilute gas of N bosons can be described with the Hamilton operator

$$H_N^U = \sum_{j=1}^N (-\Delta_j + U(x_j)) + \sum_{i<j}^N N^2 V(N(x_i - x_j))$$

acting on the Hilbert space $L_s^2(\mathbb{R}^{3N})$, the subspace of $L^2(\mathbb{R}^{3N})$ symmetric with respect to permutation of the N particles. The external potential U models the trap that confines the particles. The interaction potential V is repulsive ($V \geq 0$) and spherically symmetric; the Gross-Pitaevskii scaling $N^2 V(N \cdot)$ models rare but strong collisions. We are interested in large N (in experiments, $N \gg 10^3$).

A central role is played by the solution f to the zero-energy scattering equation

$$\left(-\Delta + \frac{1}{2}V\right)f = 0, \quad \text{with boundary condition } f(x) \rightarrow 1 \quad (|x| \rightarrow \infty).$$

Its solution has the form $f(x) \simeq 1 - a_0/|x|$ for large x , where $a_0 := (8\pi)^{-1} \int f V dx$ is the scattering length of V . By scaling, $f(N \cdot)$ solves the zero-energy scattering equation with scaled potential $N^2 V(N \cdot)$.

It was proven [LSY00] that the ground state energy E_N of the Hamiltonian H_N^U satisfies

$$\lim_{N \rightarrow \infty} \frac{E_N}{N} = \min_{\varphi \in L^2(\mathbb{R}^3), \|\varphi\|_2=1} \mathcal{E}_{\text{GP}}(\varphi), \quad (1)$$

with the Gross-Pitaevskii energy functional

$$\mathcal{E}_{\text{GP}}(\varphi) := \int dx (|\nabla \varphi|^2 + U|\varphi|^2 + 4\pi a_0 |\varphi|^4). \quad (2)$$

The ground state ψ_N^{gs} exhibits [LS02] complete Bose-Einstein condensation, in the sense

$$\gamma_{\psi_N^{\text{gs}}}^{(1)} \xrightarrow{\text{in trace norm}} |\varphi_{\text{GP}}\rangle\langle\varphi_{\text{GP}}| \quad (N \rightarrow \infty),$$

where $|\varphi_{\text{GP}}\rangle\langle\varphi_{\text{GP}}|$ is the projection on the minimizer φ_{GP} of the Gross-Pitaevskii functional (2), and $\gamma_{\psi_N^{\text{gs}}}^{(1)}$ is the one-particle reduced density matrix associated with ψ_N^{gs} , i.e. the trace-class operator on $L^2(\mathbb{R}^3)$ defined through the integral kernel

$$\gamma_{\psi_N^{\text{gs}}}^{(1)}(x; y) := \int dx_2 \dots dx_N \psi_N^{\text{gs}}(x, x_2, \dots, x_N) \overline{\psi_N^{\text{gs}}}(y, x_2, \dots, x_N).$$

Since we generally assume $\|\psi\|_2 = 1$, we have $\text{tr} \gamma_{\psi}^{(1)} = 1$.

When the traps are switched off ($U = 0$), the system starts to evolve, following the Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N^0 \psi_{N,t}, \quad \psi_{N,0} = \psi_N^{\text{gs}}.$$

It was proven [ESY10, Pic10] that $\gamma_{\psi_{N,t}}^{(1)} \rightarrow |\varphi_t\rangle\langle\varphi_t|$ as $N \rightarrow \infty$ (for any fixed $t > 0$), where φ_t is the solution to the non-linear Gross-Pitaevskii equation (here with initial data $\varphi = \varphi_{\text{GP}}$)

$$i\partial_t \varphi_t = -\Delta \varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t, \quad \varphi_0 = \varphi. \quad (3)$$

In our analysis we generalize the system to Fock space, with the advantage that we can use initial data that are superpositions of states with different numbers of particles. We introduce the bosonic Fock space $\mathcal{F} := \bigoplus_{j=0}^{\infty} L_s^2(\mathbb{R}^{3j})$ and creation/annihilation operators (more precisely operator-valued distributions) a_x^*, a_x , which create/annihilate a particle at $x \in \mathbb{R}^3$. They satisfy the canonical commutation relations $[a_x, a_y^*] = \delta(x - y)$, $[a_x^*, a_y^*] = 0 = [a_x, a_y]$. We introduce the number of particles operator $\mathcal{N} = \int dx a_x^* a_x$ and the vacuum vector $\Omega = (1, 0, \dots) \in \mathcal{F}$. On Fock space \mathcal{F} we define the Hamiltonian

$$\mathcal{H}_N := \int dx \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N} \int dx dy N^3 V(N(x - y)) a_x^* a_y^* a_y a_x. \quad (4)$$

The restriction of \mathcal{H}_N to $L_s^2(\mathbb{R}^{3N})$ coincides with the Hamiltonian H_N^0 .

For $g \in L^2(\mathbb{R}^3)$ we define the Weyl operator

$$W(g) := \exp \left(\int dx a_x^* g(x) - \text{h.c.} \right),$$

and for integral kernels $k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ we introduce the Bogoliubov transformation

$$T(k) := \exp \left(\frac{1}{2} \int dx dy k(x; y) a_x^* a_y^* - \text{h.c.} \right). \quad (5)$$

The Weyl operators have the important property of shifting the operators,

$$W^*(g)a_x^*W(g) = a_x^* + \bar{g}(x), \quad W^*(g)a_xW(g) = a_x + g(x), \quad (6)$$

whereas the Bogoliubov transformation $T(k)$ acts by

$$T^*(k)a_x^*T(k) = \int dy (a_y^* \cosh(k)(y; x) + a_y \sinh(k)(y; x)). \quad (7)$$

Here $\cosh(k)(y; x)$ and $\sinh(k)(y; x)$ are the integral kernels defined by the power series (in k) of the hyperbolic cosine/sine, with product in the sense of operators.

We will use a Weyl operator to generate a condensate. (The coherent state $W(g)\Omega$ describes a condensate with approximately $\|g\|_2^2$ particles in the one-particle state $g/\|g\|_2$.) A Bogoliubov transformation, on the other hand, is used to implement correlations among the particles. Our main result [BdS12] is the following theorem.

Theorem. *Let $V \geq 0$ and $V \in L^1 \cap L^3(\mathbb{R}^3, (1 + |x|^6)dx)$. Let $\varphi \in H^4(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$. Let $k_0(x; y) := -N(1 - f(N(x - y)))\varphi(x)\varphi(y)$. Let $\chi \in \mathcal{F}$, possibly depending on N but s. t. $\langle \chi, (\mathcal{N} + 1 + \mathcal{N}^2/N + \mathcal{H}_N)\chi \rangle$ is bounded uniform in N . We consider $\psi_{N,t} := e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\chi$, the solution to the Schrödinger equation in Fock space, i.e. $i\partial_t\psi_{N,t} = \mathcal{H}_N\psi_{N,t}$. Then there exist constants $C, c > 0$ s. t.*

$$\mathrm{tr} \left| \gamma_{\psi_{N,t}}^{(1)} - |\varphi_t\rangle\langle\varphi_t| \right| \leq \frac{C}{\sqrt{N}} \exp(c \exp(c|t|)),$$

where φ_t solves the Gross-Pitaevskii equation (3) with initial data $\varphi_0 = \varphi$.

The vector χ in the initial data describes small deviations from the squeezed coherent state $W(\sqrt{N}\varphi)T(k_0)\Omega$. The correlation structure is inserted already in the initial data; our proof keeps this structure static, showing its approximate stability. Our initial data arises naturally as an approximation to the ground state since

$$\langle W(\sqrt{N}\varphi)T(k_0)\chi, (\mathcal{H}_N + \int dx U(x)a_x^*a_x)W(\sqrt{N}\varphi)T(k_0)\chi \rangle = N\mathcal{E}_{\mathrm{GP}}(\varphi) + \mathcal{O}(N^{1/2}).$$

In our article [BdS12] we also discuss initial data with exact number of particles.

2 Strategy: Modeling correlations by a Bogoliubov transformation

The approach is inspired by the method of coherent states [RS09], developed for studying the mean-field regime. However, coherent states cannot provide a good approximation in the Gross-Pitaevskii regime because they describe completely uncorrelated states. To take into account the correlations we use Bogoliubov transformations.

For technical reasons we will compare the solution of the many-body Schrödinger equation first to the solution of the modified Gross-Pitaevskii equation

$$i\partial_t\varphi_t^{(N)} = -\Delta\varphi_t^{(N)} + (N^3f(N.)V(N.) * |\varphi_t^{(N)}|^2)\varphi_t^{(N)}, \quad \varphi_0^{(N)} = \varphi. \quad (8)$$

Since $N^3f(N.)V(N.) \rightarrow 8\pi a_0\delta$, it is easy to compare $\varphi_t^{(N)}$ with the solution φ_t of the Gross-Pitaevskii equation (3). With f the solution to the zero-energy scattering equation, let

$$k_t(x; y) := -N(1 - f(N(x - y)))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y).$$

We try to approximate the full evolution $\psi_{N,t} = e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T(k_0) \chi$ with the (up to the small deviation) squeezed coherent state $W(\sqrt{N}\varphi_t^{(N)}) T(k_t) \chi$. Thus, inspired by [RS09], we introduce the fluctuation dynamics

$$\mathcal{U}_N(t) := T^*(k_t) W^*(\sqrt{N}\varphi_t^{(N)}) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T(k_0).$$

We find the estimate

$$\text{tr} \left| \gamma_{\psi_{N,t}}^{(1)} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right| \leq \frac{C}{\sqrt{N}} \langle \mathcal{U}_N(t) \chi, \mathcal{N} \mathcal{U}_N(t) \chi \rangle. \quad (9)$$

Hence, to show the convergence of the many-body dynamics to the Gross-Pitaevskii equation, the central task is to bound the number of fluctuations $\langle \mathcal{U}_N(t) \chi, \mathcal{N} \mathcal{U}_N(t) \chi \rangle$ uniformly in N . In the next section we explain how to obtain such a bound.

3 Controlling the number of fluctuations

In this section we use the following shorthands: $W_t := W(\sqrt{N}\varphi_t^{(N)})$, $T_t := T(k_t)$, $\langle \cdot \rangle_t := \langle \mathcal{U}_N(t) \chi, \cdot \mathcal{U}_N(t) \chi \rangle$.

We intend to use Grönwall's lemma. Hence we compute the derivative

$$\partial_t \langle \mathcal{N} \rangle_t = \langle [i\mathcal{L}_N(t), \mathcal{N}] \rangle_t, \quad (10)$$

with $\mathcal{L}_N(t)$ the time-dependent generator of $\mathcal{U}_N(t)$. Explicitly

$$\mathcal{L}_N(t) = (i\partial_t T_t^*) T_t + T_t^* ((i\partial_t W_t^*) W_t + W_t^* \mathcal{H}_N W_t) T_t =: (i\partial_t T_t^*) T_t + T_t^* \mathcal{L}_N^{(0)}(t) T_t.$$

The term $(i\partial_t T_t^*) T_t$ is harmless. Let us focus on the second term. In $\mathcal{L}_N^{(0)}(t)$ we have

$$(i\partial_t W_t^*) W_t = -\sqrt{N} \int dx a_x^* i\partial_t \varphi_t^{(N)}(x) + \text{h. c.} \quad (+ \text{ irrelevant scalar}).$$

For $W_t^* \mathcal{H}_N W_t$ we use (6) and expand. We get summands which are linear in creation and annihilation operators and formally of order $N^{1/2}$; moreover quadratic summands of order one, cubics of order $N^{-1/2}$ and quartics of order N^{-1} .

Unlike in the mean-field regime [RS09], where the Hartree equation implies complete cancellation of the linear terms in $W_t^* \mathcal{H}_N W_t$ with $(i\partial_t W_t^*) W_t$, the modified Gross-Pitaevskii equation (8) leaves us with the linear, large remainder

$$N^{1/2} \int dx \left(N^3 V(N) (1 - f(N)) * |\varphi_t^{(N)}|^2 \right)(x) \varphi_t^{(N)}(x) a_x^* + \text{h. c.} \quad (11)$$

The key observation is that by conjugating $\mathcal{L}_N^{(0)}(t)$ with T_t , using (7) and expanding, we get (among many other terms) cubic terms which are not normal-ordered. Normal-ordering them by the canonical commutation relations gives rise to a linear term which cancels (11).

Similarly we get cancellations between quadratic and quartic terms of $\mathcal{L}_N^{(0)}(t)$: we conjugate them with T_t and expand the product; then normal-ordering of quartic terms gives rise to extra quadratic terms. Using the zero-energy scattering equation we now find a cancellation of some quadratic terms. (For identifying this cancellation think of $\sinh(k_t)(x; y)$ as $k_t(x; y)$ and of $\cosh(k_t)(x; y)$ as $\delta(x - y)$.)

These cancellations are crucial; they allow us to prove the operator inequality

$$[i\mathcal{L}_N(t), \mathcal{N}] \leq \mathcal{H}_N + C_t (\mathcal{N}^2/N + \mathcal{N} + 1).$$

(We denote by C_t varying constants which may grow exponentially in t (since we use bounds of the form $\|\varphi_t^{(N)}\|_{H^n} \leq Ce^{K|t|}$), but are independent of N .)

Next observe that $\mathcal{L}_N(t) = \mathcal{H}_N + \text{other terms}$, where ‘other terms’ can be bounded above and below by $\varepsilon \mathcal{H}_N$ (any $\varepsilon > 0$) and the number operator. Thus

$$\mathcal{H}_N \leq C_t (\mathcal{L}_N(t) + \mathcal{N}^2/N + \mathcal{N} + 1). \quad (12)$$

Thus we obtain $[i\mathcal{L}_N(t), \mathcal{N}] \leq C_t (\mathcal{L}_N(t) + \mathcal{N}^2/N + \mathcal{N} + 1)$. It is possible to control $\langle \mathcal{N}^2/N \rangle_t$ by $\langle (\mathcal{N} + 1)^2/N \rangle_{t=0}$ combined with $\langle \mathcal{N} \rangle_t$. This implies

$$\partial_t \langle \mathcal{N} \rangle_t \leq C_t \langle \mathcal{N} + 1 + \mathcal{L}_N(t) \rangle_t + C_t \langle (\mathcal{N} + 1)^2/N \rangle_0.$$

To close the scheme of Grönwall’s lemma, we need to control the growth of $\langle \mathcal{L}_N(t) \rangle_t$. Similar to the above estimates we find

$$\partial_t \langle \mathcal{L}_N(t) \rangle_t = \langle \dot{\mathcal{L}}_N(t) \rangle_t \leq C_t \langle \mathcal{L}_N(t) + \mathcal{N} + 1 \rangle_t + C_t \langle (\mathcal{N} + 1)^2/N \rangle_0.$$

Combining the last two bounds, we obtain (for some fixed D_t to be chosen later)

$$\partial_t \langle D_t(\mathcal{N} + 1) + \mathcal{L}_N(t) \rangle_t \leq C_t \langle D_t(\mathcal{N} + 1) + \mathcal{L}_N(t) \rangle_t + C_t \langle (\mathcal{N} + 1)^2/N \rangle_0.$$

Thus, Grönwall’s lemma implies that for some $C, c > 0$

$$\langle \mathcal{L}_N(t) + D_t(\mathcal{N} + 1) \rangle_t \leq C \exp(c \exp(ct)) \langle \mathcal{L}_N(0) + \mathcal{N} + 1 + \mathcal{N}^2/N \rangle_0.$$

By (12) there exists a $C_t > 0$ such that $\mathcal{L}_N(t) + C_t(\mathcal{N}^2/N + \mathcal{N}) \geq 0$. Choosing $D_t := C_t + 1$ we obtain

$$\langle \mathcal{N} \rangle_t \leq \langle \mathcal{L}_N(t) + D_t(\mathcal{N}^2/N + \mathcal{N}) \rangle_t \leq C \exp(c \exp(ct)),$$

which by (9) completes the proof of the main result.

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